Challenges and solutions in GW calculations for complex systems

F. Giustino, P. Umari and A. Rubio

Recent years have witnessed a tremendous improvement in the performance of high-performance scientific computing and major advances in methods for electronic structure calculations. Following this progress first-principles atomistic calculations have evolved into a discipline in its own right which could be referred to as “first-principles materials design”. In this context materials properties which depend on the electronic ground state, for instance structural parameters, elastic and vibrational properties, and the response to static electric and magnetic fields, can now be predicted with high accuracy even for large and complex systems.

However, when it comes to materials properties involving excited electronic states, established methods for ground-state calculations such as density functional theory are no longer adequate, and it becomes necessary to look for alternative theoretical approaches which are built around the concept of “electronic excitation”. Among the various methods to study such excitations the GW approximation to Hedin’s quasiparticle equations has proven very successful over the past twenty years. Besides its established predictive power in the calculation of quasiparticle band gaps, the GWmethod shows promise since it performs consistently well across widely different materials; it does not rely on adjustable parameters; and the underlying formalism is very general and non material-specific. These features make the GW method suitable for a wide class of applications, ranging from solids to molecules, bio/nano-structures, surfaces, interfaces, and defects. In addition this method is emerging as a conceptual and computational platform for developing increasingly more accurate descriptions of electronic excitations.

During June 7–10 2011 the headquarters of the Centre Européen de Calcul Atomique et Moléculaire (CECAM) in Lausanne hosted the first international CECAM/Psi-k workshop entirely devoted to the GW method and its applications in condensed matter physics and nanoscience. This workshop gathered over 50 experts in the area of electronic excitations from 13 Countries across the globe, and showed that many research groups are currently investing into the development and application of the GW method. Both oral and poster presentations demonstrated that this approach is becoming ubiquitous in the study of electronic excitations, and finds an extremely diverse range of applications, spanning photoelectron spectroscopy, energetic of defects, molecular electronics and spintronics, as well as strongly-correlated systems. During this workshop it was also clear that significant efforts are being made to explore alternative approaches to GW calculations, including selfconsistent calculations, calculations of total energies, calculations without unoccupied states, and all-electron calculations.

The present issue “Challenges and solutions in GW calculations for complex systems” collects contributions from key presentations of this CECAM/Psi-k workshop, and tries to reflect the breadth of the current research in electronic structure calculations based on the GW method, on both fronts of applications and methodology.

The contributions cover:
– the analysis of plasmon-pole models in G0W0 calculations
– the development of GW methods based on efficient local orbital basis sets
– the validation and use of the G0W0 method for accurate calculations of orbital energies in organic molecules
– the assessment of the performance of hybrid methods based on the GW approximation for magnetic and strongly-correlated systems
– the extension of the GW method to the calculation of plasmon satellites in valence photoemission spectroscopy
– the inclusion of quantum nuclear effects in the calculation of quasiparticle energies.

We hope that the present Special Issue of the European Physical Journal B will provide an exciting perspective on the current state-of-the-art in this vast and fascinating research area, and encourage further work towards developing new and more efficient GW approaches in view of addressing the widest range of materials and their properties.